Magnetism and Electron Correlations in Iron Pnictides

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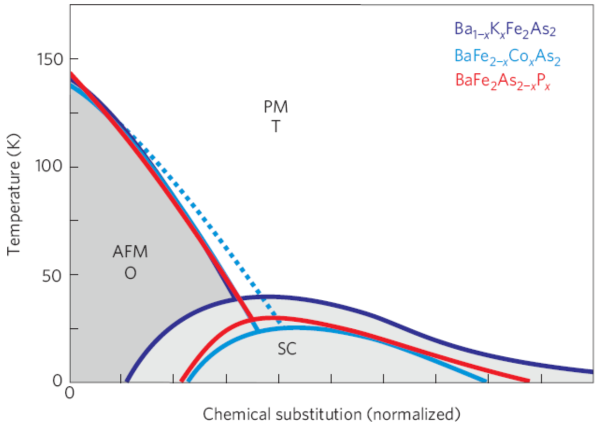
G. F. Chen	**N. L. Wang**	**H. A. Mook**
P. C. Dai	**H. Wang**	**L. L. Zhao**
M. D. Jones	**E. Morosan**	**M. H. Fang**

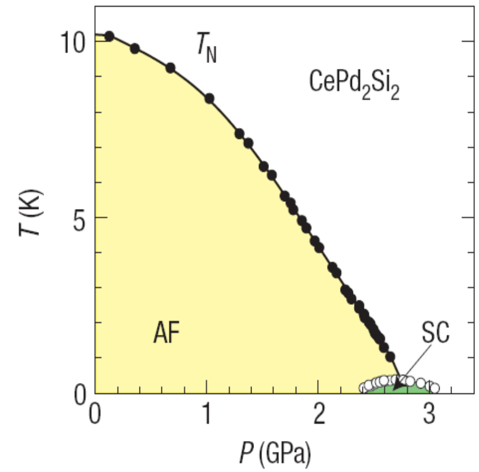
Superconductivity at the border of magnetism

Iron pnictides



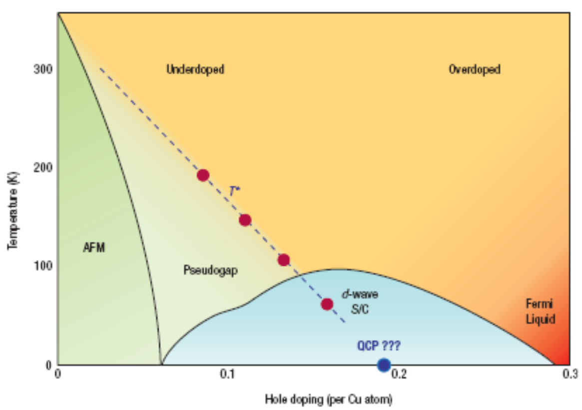
Paglione & Greene

Heavy fermions



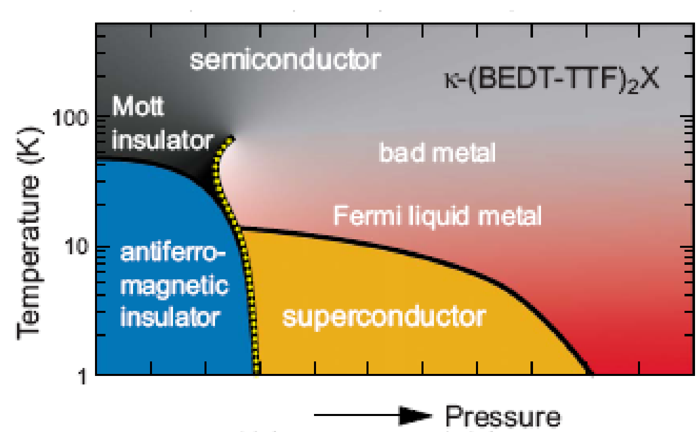
Mathur et al

Cuprates



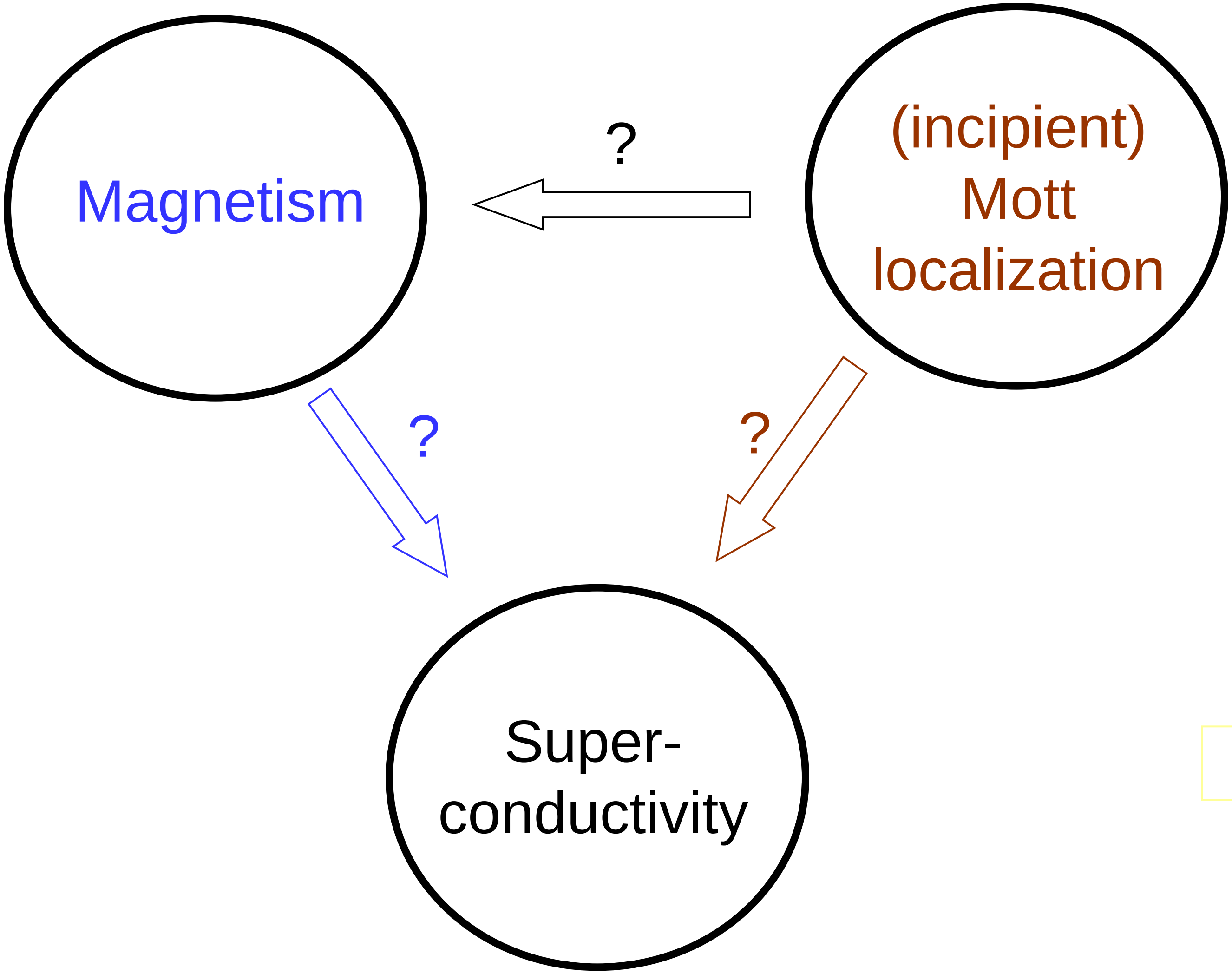
Broun

Organics

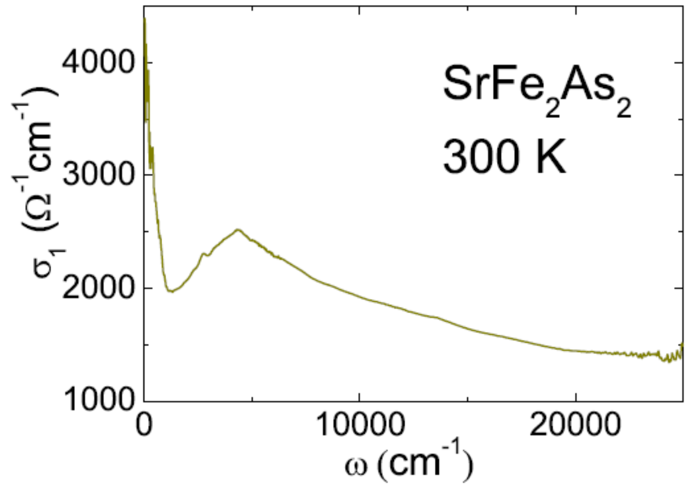


Faltermeier et al

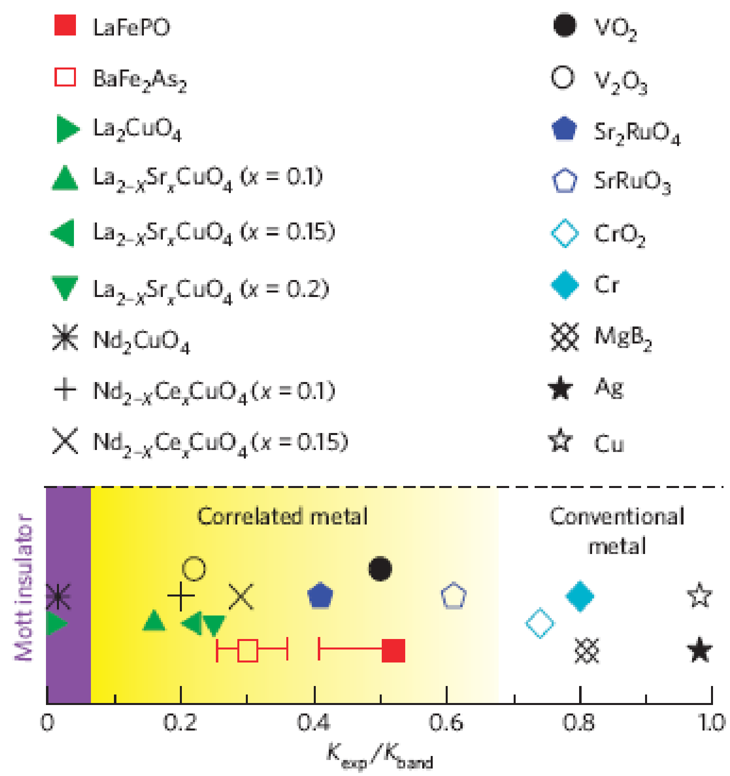
Magnetism, Localization, and Superconductivity



Iron pnictides as bad metals



W. Z. Hu et al, PRL 101, 257005 ('08)



Also

Resistivity @ room temperature

Like V_2O_3 ,

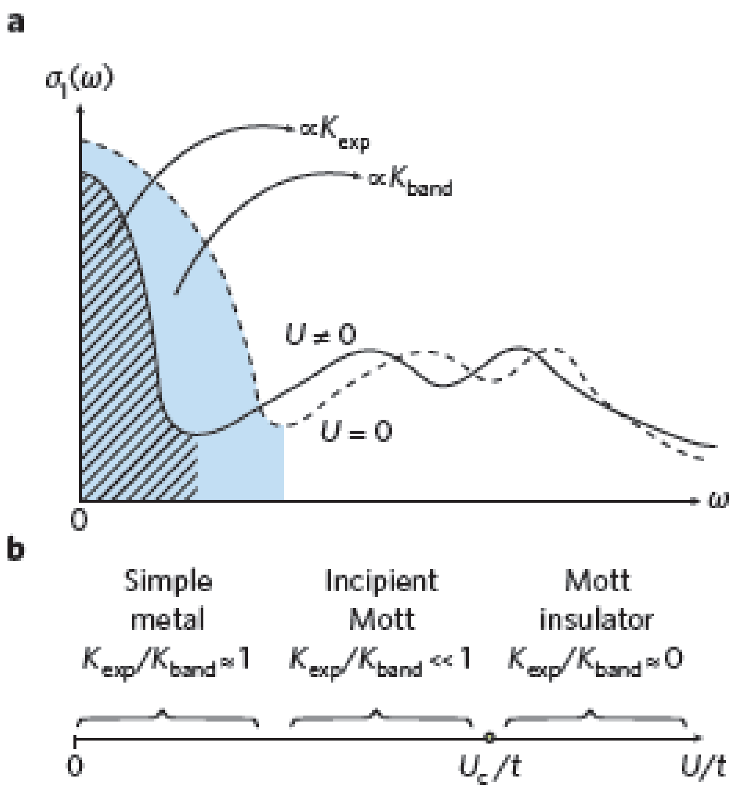
quite unlike Cr

M. M. Qazilbash et al,

Nature Phys. 5, 647 ('09);

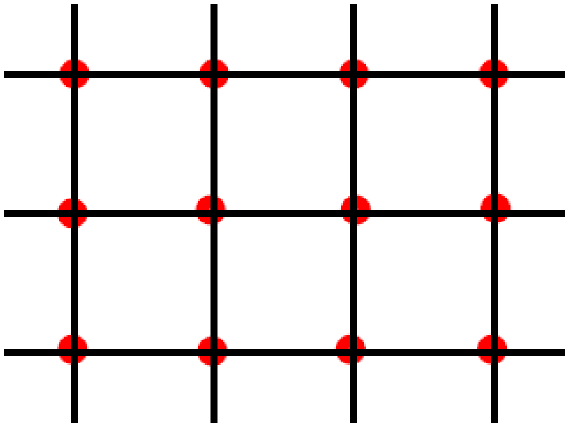
L. Degiorgi, arXiv:1006.4698

Push it over the edge,
to the Mott localized side



R. Yu and QS,
arXiv: 1006.2337 ('10)

$La_2O_3Fe_2Se_2$

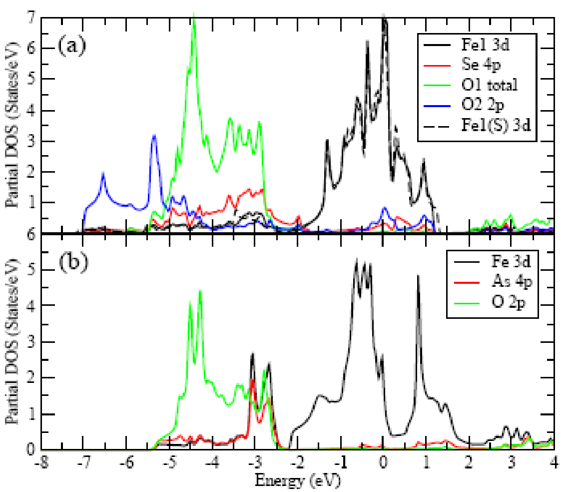


- **Fe square lattice**
- **Expanded lattice**
- **D-band narrowing**
- **Mott insulator**

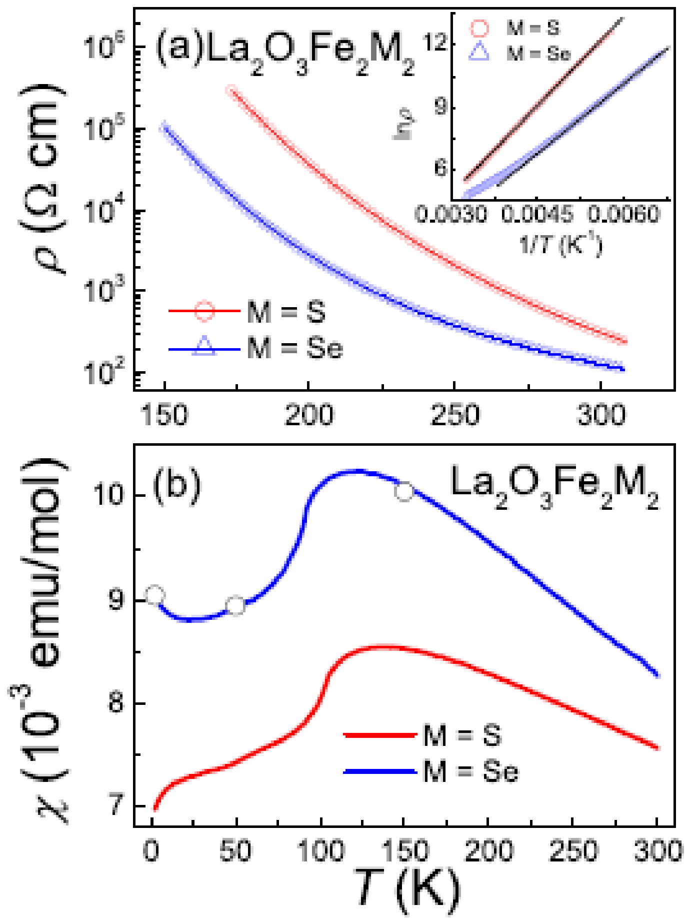
J.-X. Zhu, R. Yu et al,
PRL 104, 216405 ('10)

Push it over the edge, to the Mott localized side

$La_2O_3Fe_2Se_2$



LaFeAsO



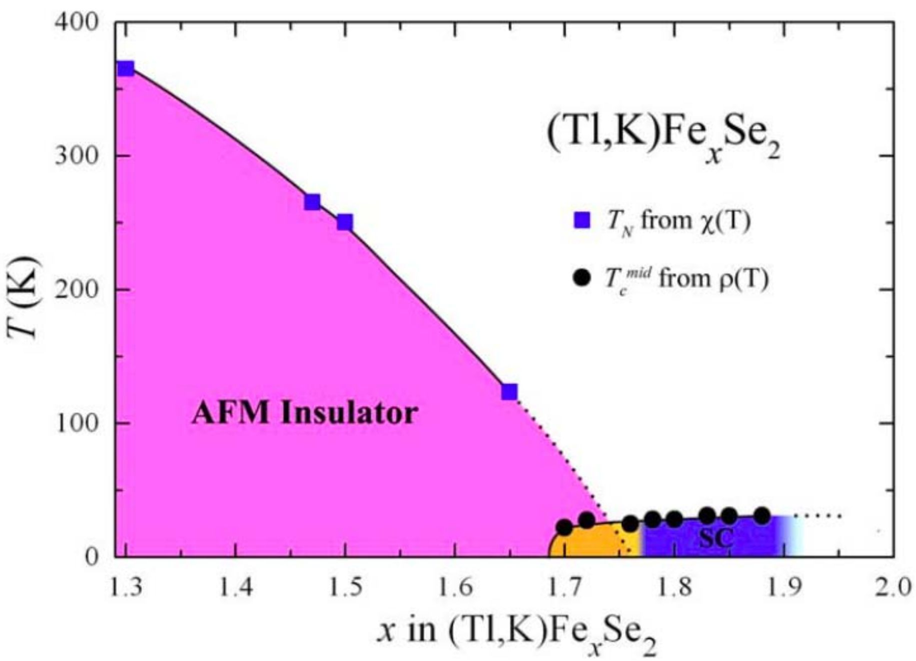
d-electron band narrowing

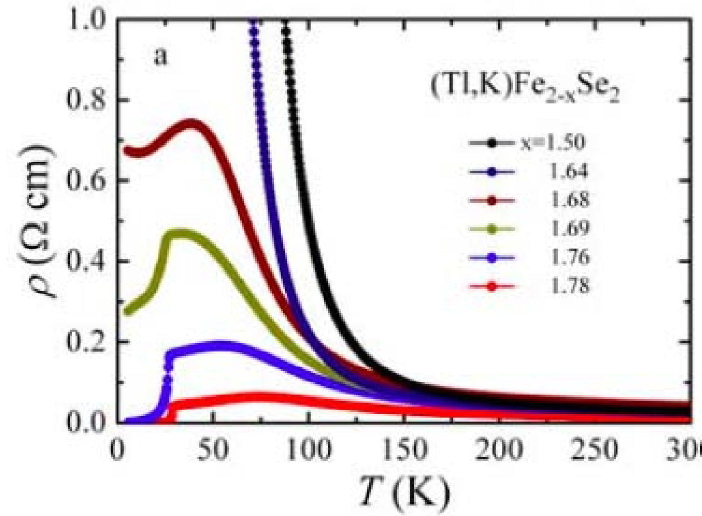
Evidence for Mott insulator

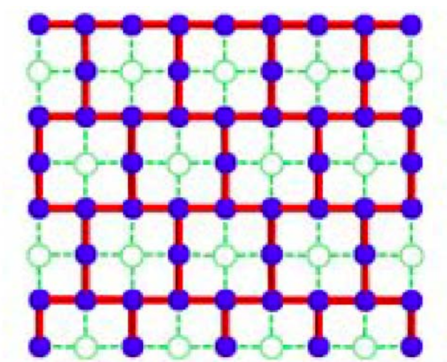
J. X. Zhu, R. Yu, H. Wang, L. L. Zhao, M. D. Jones, J. Dai, E. Abrahams, E. Morosan, M. Fang, QS, PRL 104, 216405 ('10)

Insulating AFM as Parents to SC KFeSe?

$(K,Tl)Fe_xSe_2$

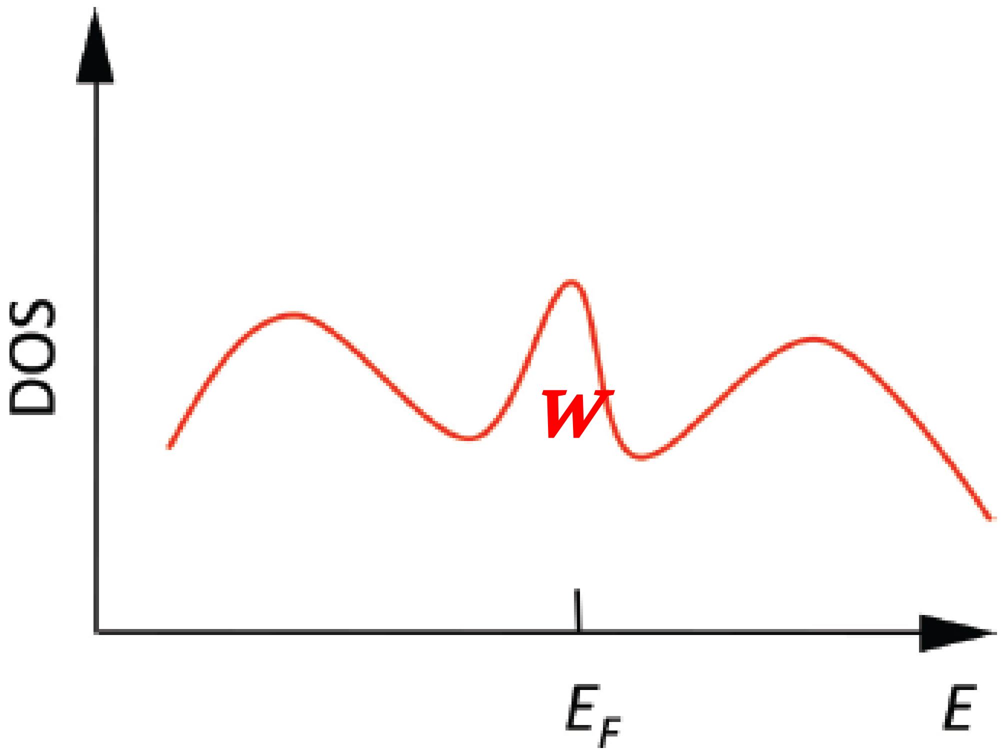






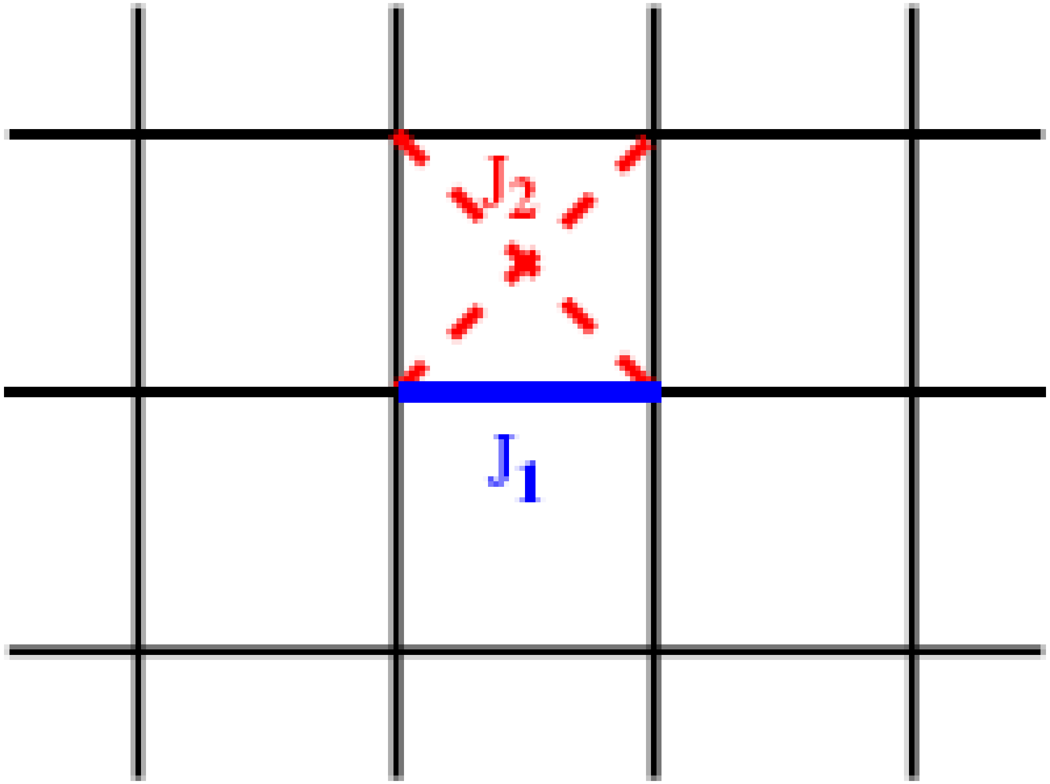
M. Fang et al, arXiv:1012.5236 ('10)

Proximity to Mott transition



- **Precursors to the lower and upper Hubbard bands – incoherent features.**
- **Use *w* as small parameter, instead of *U/t***

J_1-J_2 Frustration & Antiferromagnetism



$J_2 >\sim J_1 / 2$

QS & E. Abrahams,
PRL 101, 076401 (2008)

See also Ab initio calculations:

T. Yildirim; F. Ma et al;
Z. P. Yin et al

Spin spectral weight

Fermi surfaces are small pockets:

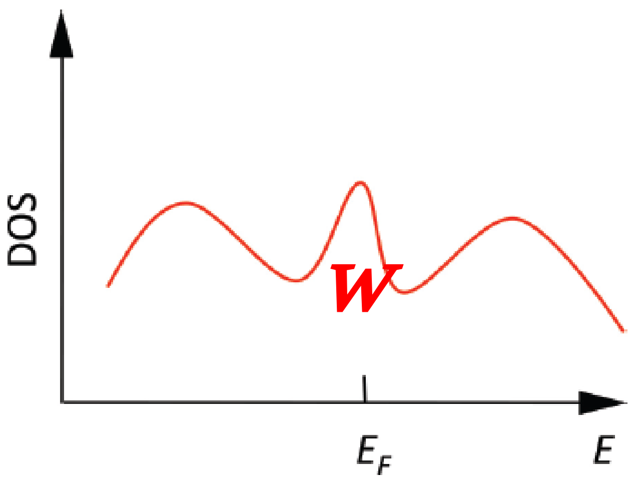
Difficult to get ~1.0 μ_B/Fe from electrons near the Fermi surfaces alone

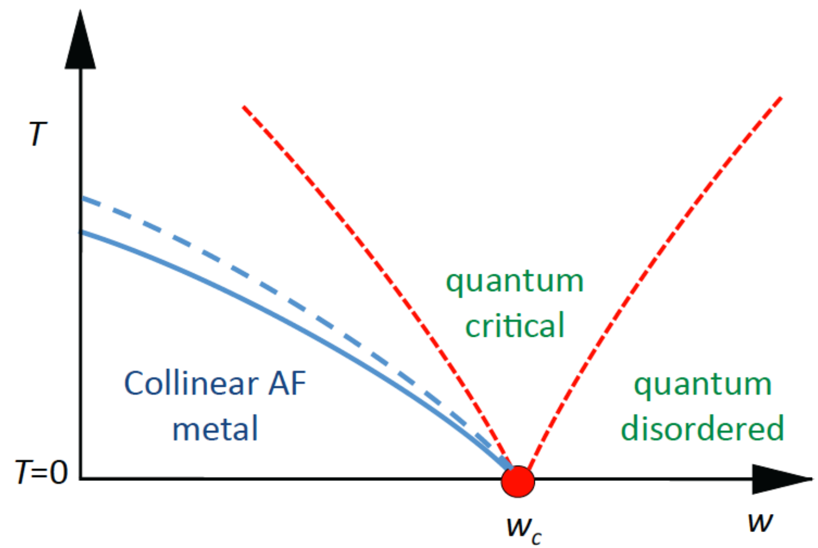
Quantum Criticality in Iron Pnictides

$$\mathcal{S} = \int d\mathbf{q} \int d\omega \left[(r + \omega^2 + c\mathbf{q}^2)((\mathbf{m})^2 + (\mathbf{m}')^2) + v(q_x^2 - q_y^2)\mathbf{m}\cdot\mathbf{m}' \right]$$

$$+ \int \left[u(\mathbf{m})^4 + u(\mathbf{m}')^4 + \tilde{u}(\mathbf{m}\cdot\mathbf{m}')^2 + u'(\mathbf{m})^2(\mathbf{m}')^2 \right] + \ldots,$$

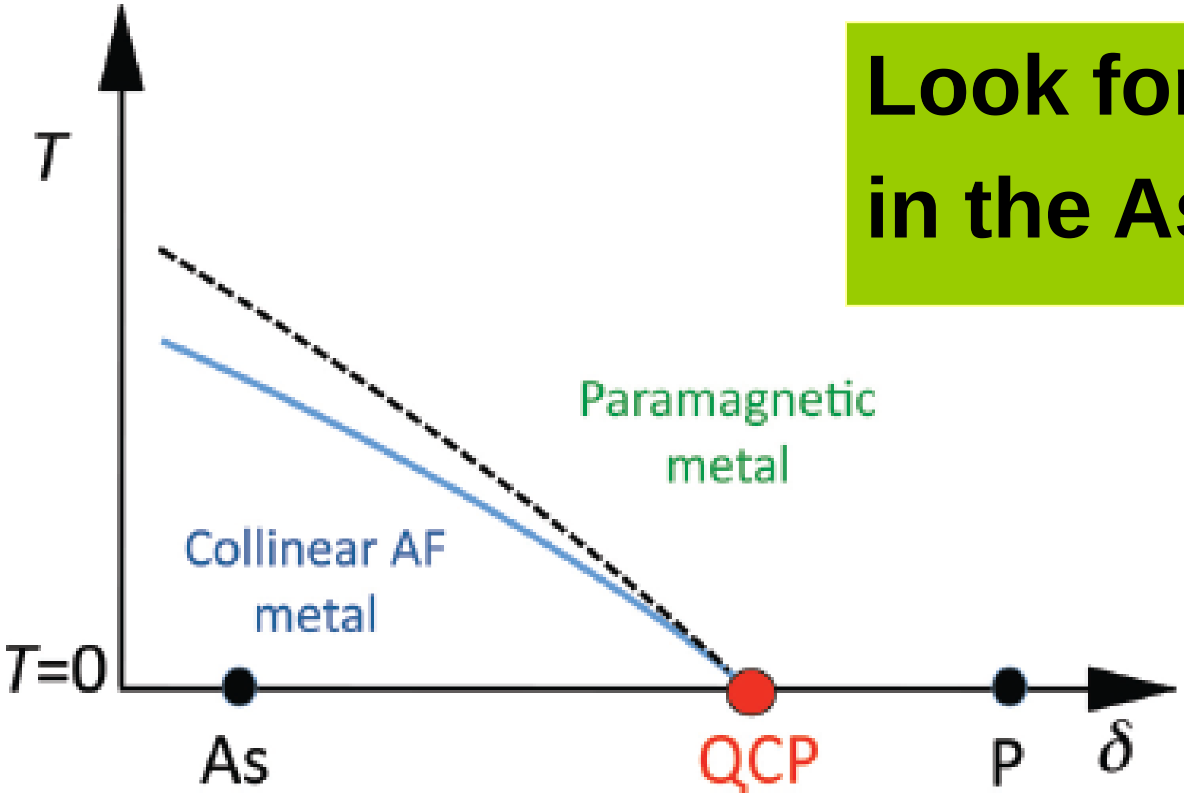
$$\Delta\mathcal{S} = \int d\mathbf{q} \int d\omega (wA_{\mathbf{Q}} + \gamma|\omega|) \left[(\mathbf{m})^2 + (\mathbf{m}')^2 \right]$$





J. Dai, QS, J-X Zhu & E. Abrahams, PNAS 106, 4118 ('09);
QS, E. Abrahams, J. Dai & J-X Zhu, NJP 11, 045001 ('09)

Quantum Critical Point through isoelectronic P/As doping

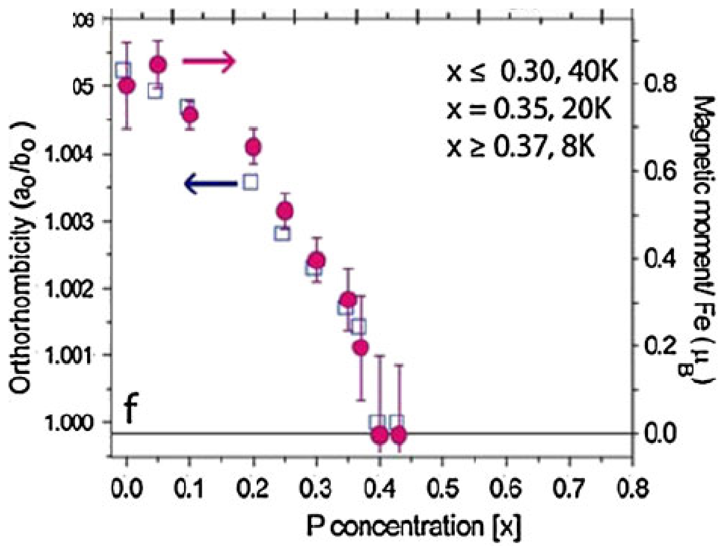


Look for QCP in the $As_{1-x}P_x$ series

J. Dai, QS, J-X Zhu & E. Abrahams, PNAS 106, 4118 ('09)

Quantum Critical Point in the $As_{1-x}P_x$ series

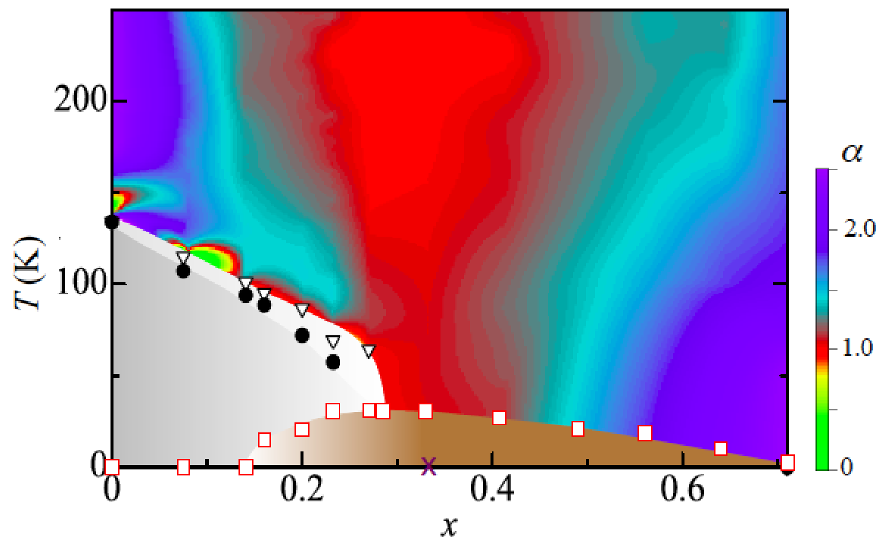
$CeFeAs_{1-x}P_xO$



C. de la Cruz et al, PRL 104, 017204 (2010)

see also Y. Luo et al; A. Jesche et al

$BaFe_2(As_{1-x}P_x)_2$

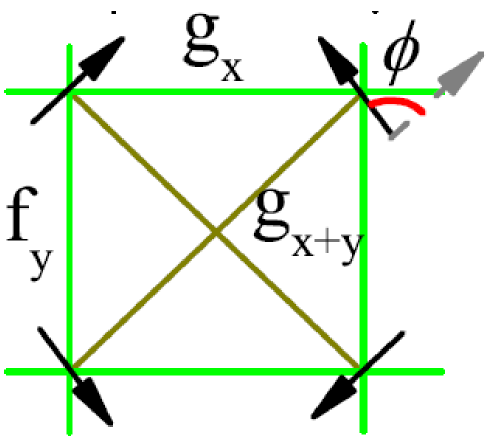


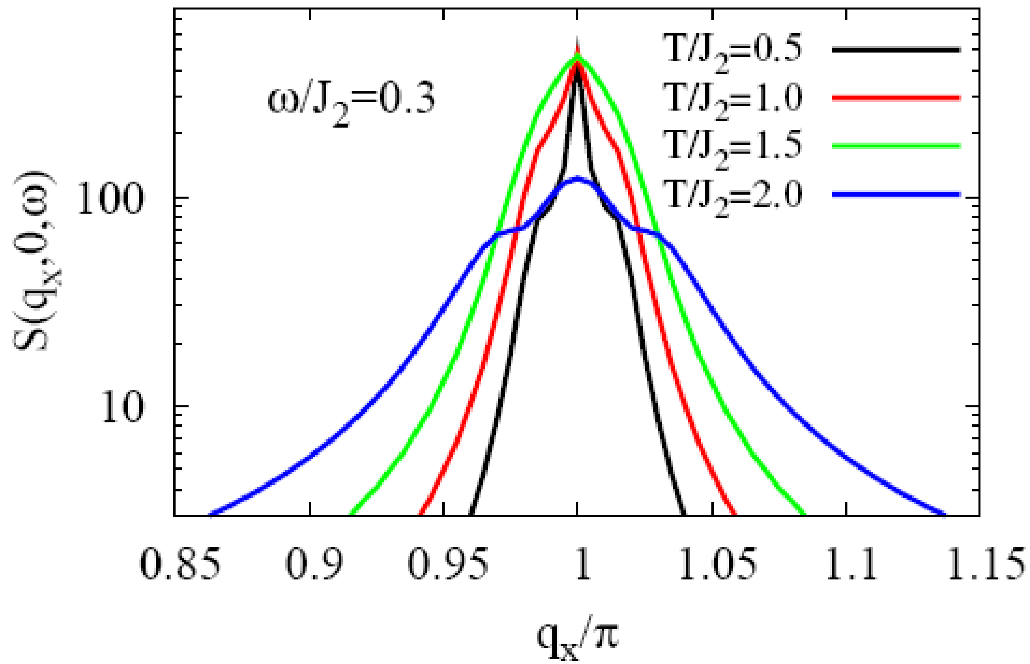
S. Kasahara et al, PRB 81, 184519 ('10)

see also S. Jiang et al, JPCM ('09)

Spin dynamics in the paramagnetic phase of parent arsenides

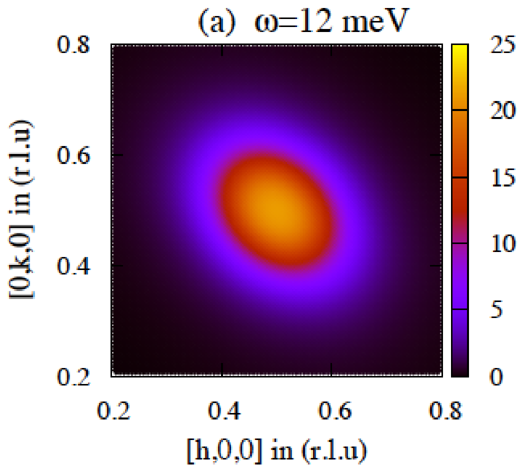
$$H = J_1 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

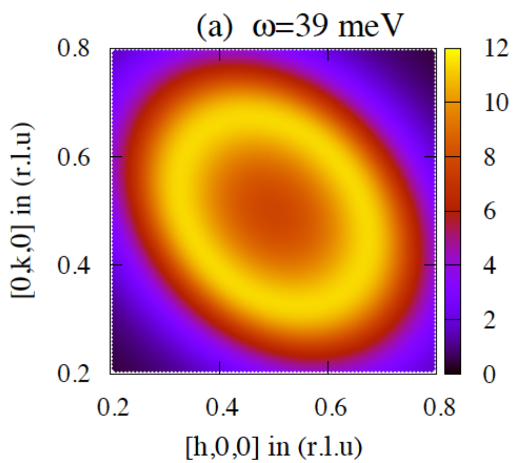


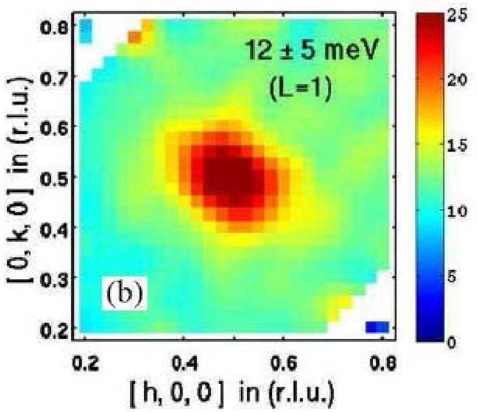


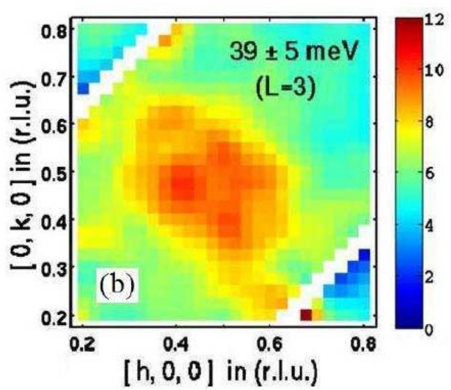
P. Goswami, R. Yu, QS
& E. Abrahams, arXiv:1009.1111

Spin dynamics in the paramagnetic phase of parent arsenides









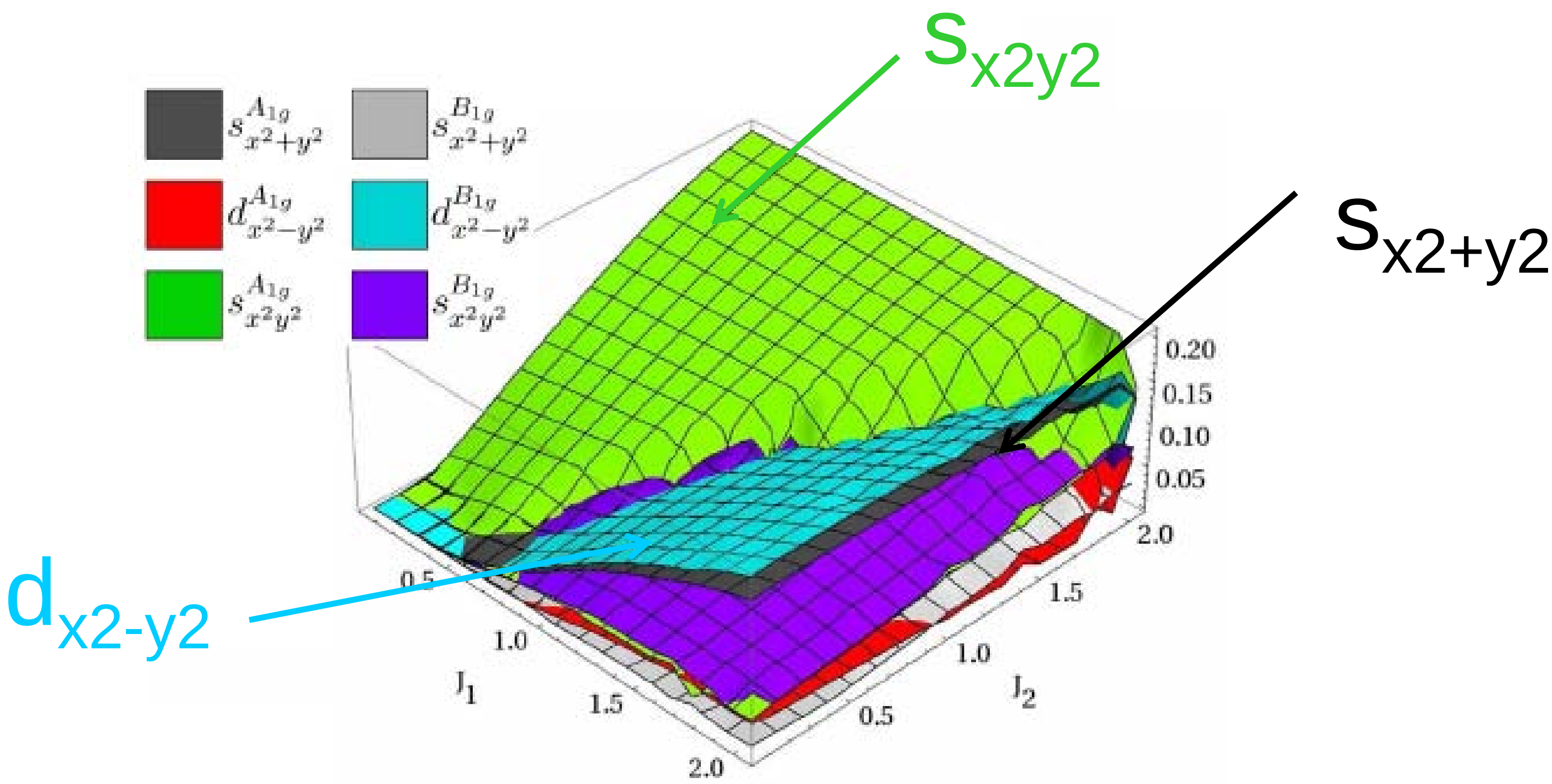
P. Goswami, R. Yu, QS
& E. Abrahams, arXiv:1009.1111

Expts: S. O. Diallo et al, PRB 81 ('10)

Superconductivity in multiband t-J_1-J_2 model

- When J_1-J_2 dominates, and with magnetic frustration ($J_1 \sim J_2$): degeneracy among s_{x2y2}, d_{xy}; and d_{x2-y2}, s_{x2+y2}
- Kinetic energy breaks degeneracy, and could favor either extended s-wave or d wave

P. Goswami, P. Nikolic, & QS, EPL 91, 37006 (2010)



P. Goswami, P. Nikolic,
& QS, EPL 91, 37006 (2010)

Cf. Evidence for different pairing states in different pnictides.

Eg, P-doped BaFe2As2 vs K-doped BaFe2As2,

K. Hashimoto et al, PRB81, 220501 (’10)

Y. Nakai et al, PRB 81, 020503 (’10);

J. S. Kim et al, arXiv:1002.3355.

SUMMARY

- **Iron pnictides are bad metals**
- **Parent iron arsenides are suggested to be close to a Mott transition**
- **Pushed to the Mott side by band narrowing, as in $La_2O_3Fe_2Se_2$**

SUMMARY

- **Iron pnictides are bad metals**
- **Parent iron arsenides are suggested to be close to a Mott transition**
- **Pushed to the Mott side by band narrowing, as in $La_2O_3Fe_2Se_2$**
- **Incoh. electronic excitations → quasi-local moments: J_1-J_2 magnetic frustration; anisotropic dynamics**
- **Magnetic quantum critical point, by varying degree of itinerancy via isoelectronic doping**
- **Quasi-degeneracy of supercond. pairing states**